

ORGANOMETALLICS

Organometallics, 1996, 15(9), 2410-2412, DOI:[10.1021/om960007i](https://doi.org/10.1021/om960007i)

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L2412-1

Table 1. Crystal data and structure refinement for 95144.

Empirical formula	$C_{10}H_{14.50}Ti_{0.50}$
Formula weight	158.67
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	$a = 13.8225(6)$ Å $\alpha = 90^\circ$ $b = 9.7919(4)$ Å $\beta = 103.2110(10)^\circ$ $c = 13.6055(6)$ Å $\gamma = 90^\circ$
Volume	1792.75(13) Å ³
Z	8
Density (calculated)	1.176 Mg/m ³
Absorption coefficient	0.470 mm ⁻¹
F(000)	684
Crystal size	0.50 x 0.50 x 0.35 mm
θ range for data collection	2.57 to 24.98°
Index ranges	$-14 \leq h \leq 16$, $-11 \leq k \leq 10$, $-13 \leq l \leq 16$
Reflections collected	4469
Independent reflections	1562 ($R_{int} = 0.0269$)
Absorption correction	Semi-empirical
Max. and min. transmission	0.63306 and 0.56184
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1562 / 105 / 200
Goodness-of-fit on F^2	1.043
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0328$, $wR2 = 0.0904$
R indices (all data)	$R1 = 0.0358$, $wR2 = 0.0934$
Extinction coefficient	0.0058(9)
Largest diff. peak and hole	0.167 and -0.229 eÅ ⁻³

L2412-2

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 95144. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
Ti(1)	2374(1)	2398(1)	4658(1)	34(1)	0.50
C(11)	2883(4)	1200(5)	3606(4)	32(1)	0.50
C(12)	3724(8)	2055(9)	4000(6)	33(2)	0.50
C(13)	4142(9)	1736(17)	5022(12)	34(3)	0.50
C(14)	3611(8)	618(11)	5326(7)	37(4)	0.50
C(15)	2847(8)	248(9)	4418(8)	33(2)	0.50
C(16)	1983(12)	1767(16)	3001(11)	48(3)	0.50
C(17)	4066(12)	3319(13)	3492(13)	69(4)	0.50
C(18)	5056(9)	2280(14)	5755(10)	63(4)	0.50
C(19)	3798(11)	-267(12)	6274(8)	52(4)	0.50
C(20)	2016(10)	-790(10)	4330(10)	51(2)	0.50
C(11A)	2227(4)	3450(5)	6149(4)	35(1)	0.50
C(12A)	1331(7)	2688(9)	5777(7)	31(1)	0.50
C(13A)	856(10)	3320(18)	4857(12)	33(3)	0.50
C(14A)	1461(7)	4434(9)	4706(7)	36(4)	0.50
C(15A)	2305(8)	4508(9)	5449(8)	34(2)	0.50
C(16A)	2962(11)	3200(18)	7140(11)	53(3)	0.50
C(17A)	943(11)	1640(17)	6377(13)	74(4)	0.50
C(18A)	-123(8)	2805(11)	4231(8)	43(3)	0.50
C(19A)	1118(12)	5250(14)	3749(9)	58(4)	0.50
C(20A)	3067(12)	5577(13)	5509(11)	86(5)	0.50

L2412-3 3

Table 3. Bond lengths [Å] and angles [°] for 95144.

Ti(1)-C(11)	2.093(4)	Ti(1)-C(15)	2.250(8)
Ti(1)-C(12)	2.272(8)	Ti(1)-C(16)	2.281(14)
Ti(1)-C(11A)	2.325(4)	Ti(1)-C(15A)	2.342(8)
Ti(1)-C(12A)	2.340(7)	Ti(1)-C(13A)	2.36(2)
Ti(1)-C(14A)	2.368(10)	Ti(1)-C(14)	2.465(10)
Ti(1)-C(13)	2.467(14)	C(11)-C(12)	1.433(11)
C(11)-C(16)	1.437(14)	C(11)-C(15)	1.455(11)
C(12)-C(13)	1.413(14)	C(12)-C(17)	1.543(11)
C(13)-C(14)	1.431(14)	C(13)-C(18)	1.517(13)
C(14)-C(15)	1.475(12)	C(14)-C(19)	1.527(11)
C(15)-C(20)	1.518(12)	C(16)-H(16B)	0.99
C(16)-H(16C)	0.99	C(17)-H(17A)	0.98
C(17)-H(17B)	0.98	C(17)-H(17C)	0.98
C(18)-H(18A)	0.98	C(18)-H(18B)	0.98
C(18)-H(18C)	0.98	C(19)-H(19A)	0.98
C(19)-H(19B)	0.98	C(19)-H(19C)	0.98
C(20)-H(20A)	0.98	C(20)-H(20B)	0.98
C(20)-H(20C)	0.98	C(11A)-C(15A)	1.428(11)
C(11A)-C(12A)	1.435(10)	C(11A)-C(16A)	1.510(13)
C(12A)-C(13A)	1.416(14)	C(12A)-C(17A)	1.486(13)
C(13A)-C(14A)	1.417(14)	C(13A)-C(18A)	1.511(13)
C(14A)-C(15A)	1.360(13)	C(14A)-C(19A)	1.509(12)
C(15A)-C(20A)	1.474(13)	C(16A)-H(16D)	0.98
C(16A)-H(16E)	0.98	C(16A)-H(16F)	0.98
C(17A)-H(17G)	0.98	C(17A)-H(17H)	0.98
C(17A)-H(17I)	0.98	C(18A)-H(18G)	0.98
C(18A)-H(18H)	0.98	C(18A)-H(18I)	0.98
C(19A)-H(19G)	0.98	C(19A)-H(19H)	0.98
C(19A)-H(19I)	0.98	C(20A)-H(20G)	0.98
C(20A)-H(20H)	0.98	C(20A)-H(20I)	0.98
C(11)-Ti(1)-C(15)	38.9(3)	C(11)-Ti(1)-C(12)	38.1(2)
C(15)-Ti(1)-C(12)	60.8(3)	C(11)-Ti(1)-C(16)	38.1(4)
C(15)-Ti(1)-C(16)	67.3(4)	C(12)-Ti(1)-C(16)	66.4(5)
C(11)-Ti(1)-C(11A)	162.8(3)	C(15)-Ti(1)-C(11A)	128.8(3)
C(12)-Ti(1)-C(11A)	130.7(3)	C(16)-Ti(1)-C(11A)	159.2(4)
C(11)-Ti(1)-C(15A)	149.8(3)	C(15)-Ti(1)-C(15A)	159.4(6)
C(12)-Ti(1)-C(15A)	115.8(3)	C(16)-Ti(1)-C(15A)	131.9(5)
C(11A)-Ti(1)-C(15A)	35.6(3)	C(11)-Ti(1)-C(12A)	150.0(3)
C(15)-Ti(1)-C(12A)	116.8(3)	C(12)-Ti(1)-C(12A)	163.3(5)
C(16)-Ti(1)-C(12A)	129.4(5)	C(11A)-Ti(1)-C(12A)	35.8(2)
C(15A)-Ti(1)-C(12A)	59.9(3)	C(11)-Ti(1)-C(13A)	137.8(4)
C(15)-Ti(1)-C(13A)	132.2(5)	C(12)-Ti(1)-C(13A)	159.3(5)
C(16)-Ti(1)-C(13A)	101.6(5)	C(11A)-Ti(1)-C(13A)	58.2(4)
C(15A)-Ti(1)-C(13A)	58.5(5)	C(12A)-Ti(1)-C(13A)	35.1(4)
C(11)-Ti(1)-C(14A)	139.0(3)	C(15)-Ti(1)-C(14A)	165.0(4)
C(12)-Ti(1)-C(14A)	128.8(3)	C(16)-Ti(1)-C(14A)	104.4(4)
C(11A)-Ti(1)-C(14A)	56.6(3)	C(15A)-Ti(1)-C(14A)	33.6(3)
C(12A)-Ti(1)-C(14A)	57.9(3)	C(13A)-Ti(1)-C(14A)	34.9(4)
C(11)-Ti(1)-C(14)	62.8(3)	C(15)-Ti(1)-C(14)	36.1(3)
C(12)-Ti(1)-C(14)	58.5(4)	C(16)-Ti(1)-C(14)	99.2(4)
C(11A)-Ti(1)-C(14)	100.5(3)	C(15A)-Ti(1)-C(14)	123.5(4)
C(12A)-Ti(1)-C(14)	108.9(4)	C(13A)-Ti(1)-C(14)	142.1(5)
C(14A)-Ti(1)-C(14)	156.1(4)	C(11)-Ti(1)-C(13)	61.1(4)
C(15)-Ti(1)-C(13)	58.4(4)	C(12)-Ti(1)-C(13)	34.4(4)
C(16)-Ti(1)-C(13)	97.3(5)	C(11A)-Ti(1)-C(13)	102.8(4)
C(15A)-Ti(1)-C(13)	106.4(5)	C(12A)-Ti(1)-C(13)	129.1(5)
C(13A)-Ti(1)-C(13)	161.0(8)	C(14A)-Ti(1)-C(13)	136.5(5)
C(14)-Ti(1)-C(13)	33.7(4)	C(12)-C(11)-C(16)	120.7(9)

L2412-4

C(12)-C(11)-C(15)	104.8(7)	C(16)-C(11)-C(15)	120.5(10)
C(12)-C(11)-Ti(1)	77.8(3)	C(16)-C(11)-Ti(1)	78.1(6)
C(15)-C(11)-Ti(1)	76.4(3)	C(13)-C(12)-C(11)	110.6(8)
C(13)-C(12)-C(17)	121.3(11)	C(11)-C(12)-C(17)	127.3(10)
C(13)-C(12)-Ti(1)	80.4(7)	C(11)-C(12)-Ti(1)	64.2(4)
C(17)-C(12)-Ti(1)	114.9(8)	C(12)-C(13)-C(14)	109.4(9)
C(12)-C(13)-C(18)	131.4(11)	C(14)-C(13)-C(18)	118.9(12)
C(12)-C(13)-Ti(1)	65.3(6)	C(14)-C(13)-Ti(1)	73.1(6)
C(18)-C(13)-Ti(1)	132.7(12)	C(13)-C(14)-C(15)	105.2(9)
C(13)-C(14)-C(19)	132.8(10)	C(15)-C(14)-C(19)	121.3(10)
C(13)-C(14)-Ti(1)	73.2(6)	C(15)-C(14)-Ti(1)	64.0(5)
C(19)-C(14)-Ti(1)	133.0(8)	C(11)-C(15)-C(14)	109.7(8)
C(11)-C(15)-C(20)	121.7(9)	C(14)-C(15)-C(20)	127.9(10)
C(11)-C(15)-Ti(1)	64.7(4)	C(14)-C(15)-Ti(1)	79.9(6)
C(20)-C(15)-Ti(1)	113.5(7)	C(11)-C(16)-Ti(1)	63.9(5)
C(11)-C(16)-H(16B)	117.4(8)	Ti(1)-C(16)-H(16B)	117.4(5)
C(11)-C(16)-H(16C)	117.4(8)	Ti(1)-C(16)-H(16C)	117.4(5)
H(16B)-C(16)-H(16C)	114.4	C(12)-C(17)-H(17A)	109.5(7)
C(12)-C(17)-H(17B)	109.5(7)	H(17A)-C(17)-H(17B)	109.5
C(12)-C(17)-H(17C)	109.5(7)	H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5	C(13)-C(18)-H(18A)	109.5(8)
C(13)-C(18)-H(18B)	109.5(8)	H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5(8)	H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5	C(14)-C(19)-H(19A)	109.5(6)
C(14)-C(19)-H(19B)	109.5(7)	H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5(6)	H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5	C(15)-C(20)-H(20A)	109.5(6)
C(15)-C(20)-H(20B)	109.5(6)	H(20A)-C(20)-H(20B)	109.5
C(15)-C(20)-H(20C)	109.5(6)	H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5	C(15A)-C(11A)-C(12A)	109.4(7)
C(15A)-C(11A)-C(16A)	125.1(10)	C(12A)-C(11A)-C(16A)	125.5(10)
C(15A)-C(11A)-Ti(1)	72.8(4)	C(12A)-C(11A)-Ti(1)	72.7(3)
C(16A)-C(11A)-Ti(1)	122.1(7)	C(13A)-C(12A)-C(11A)	105.9(9)
C(13A)-C(12A)-C(17A)	129.4(11)	C(11A)-C(12A)-C(17A)	123.7(10)
C(13A)-C(12A)-Ti(1)	73.1(8)	C(11A)-C(12A)-Ti(1)	71.5(3)
C(17A)-C(12A)-Ti(1)	128.8(9)	C(12A)-C(13A)-C(14A)	107.1(9)
C(12A)-C(13A)-C(18A)	121.8(12)	C(14A)-C(13A)-C(18A)	131.1(12)
C(12A)-C(13A)-Ti(1)	71.8(7)	C(14A)-C(13A)-Ti(1)	73.0(7)
C(18A)-C(13A)-Ti(1)	120.9(11)	C(15A)-C(14A)-C(13A)	111.6(9)
C(15A)-C(14A)-C(19A)	131.3(9)	C(13A)-C(14A)-C(19A)	117.0(11)
C(15A)-C(14A)-Ti(1)	72.2(5)	C(13A)-C(14A)-Ti(1)	72.1(8)
C(19A)-C(14A)-Ti(1)	119.1(8)	C(14A)-C(15A)-C(11A)	105.9(8)
C(14A)-C(15A)-C(20A)	124.1(11)	C(11A)-C(15A)-C(20A)	129.8(10)
C(14A)-C(15A)-Ti(1)	74.3(6)	C(11A)-C(15A)-Ti(1)	71.5(4)
C(20A)-C(15A)-Ti(1)	123.3(7)	C(11A)-C(16A)-H(16D)	109.5(6)
C(11A)-C(16A)-H(16E)	109.5(8)	H(16D)-C(16A)-H(16E)	109.5
C(11A)-C(16A)-H(16F)	109.5(7)	H(16D)-C(16A)-H(16F)	109.5
H(16E)-C(16A)-H(16F)	109.5	C(12A)-C(17A)-H(17G)	109.5(8)
C(12A)-C(17A)-H(17H)	109.5(7)	H(17G)-C(17A)-H(17H)	109.5
C(12A)-C(17A)-H(17I)	109.5(8)	H(17G)-C(17A)-H(17I)	109.5
H(17H)-C(17A)-H(17I)	109.5	C(13A)-C(18A)-H(18G)	109.5(8)
C(13A)-C(18A)-H(18H)	109.5(7)	H(18G)-C(18A)-H(18H)	109.5
C(13A)-C(18A)-H(18I)	109.5(8)	H(18G)-C(18A)-H(18I)	109.5
H(18H)-C(18A)-H(18I)	109.5	C(14A)-C(19A)-H(19G)	109.5(7)
C(14A)-C(19A)-H(19H)	109.5(6)	H(19G)-C(19A)-H(19H)	109.5
C(14A)-C(19A)-H(19I)	109.5(7)	H(19G)-C(19A)-H(19I)	109.5
H(19H)-C(19A)-H(19I)	109.5	C(15A)-C(20A)-H(20G)	109.5(7)
C(15A)-C(20A)-H(20H)	109.5(7)	H(20G)-C(20A)-H(20H)	109.5
C(15A)-C(20A)-H(20I)	109.5(8)	H(20G)-C(20A)-H(20I)	109.5
H(20H)-C(20A)-H(20I)	109.5		

Symmetry transformations used to generate equivalent atoms:

L2412-5 5

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 95144.2. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(h a)^2 U_{11} + \dots + 2 h k a b U_{12}]$

	U11	U22	U33	U23	U13	U12
Ti (1)	28 (1)	45 (1)	28 (1)	-5 (1)	3 (1)	7 (1)
C (11)	35 (2)	36 (3)	25 (2)	-9 (2)	7 (2)	5 (2)
C (12)	38 (2)	42 (4)	23 (3)	-3 (2)	13 (2)	2 (2)
C (13)	21 (5)	35 (4)	50 (7)	-3 (4)	13 (4)	-3 (3)
C (14)	28 (4)	50 (6)	26 (5)	-11 (4)	-8 (3)	13 (3)
C (15)	24 (3)	34 (3)	43 (3)	-6 (2)	12 (2)	7 (2)
C (16)	52 (5)	54 (4)	37 (4)	-1 (3)	7 (3)	15 (3)
C (17)	68 (7)	60 (5)	85 (7)	36 (4)	26 (6)	-11 (4)
C (18)	34 (5)	90 (7)	68 (7)	4 (5)	15 (4)	9 (4)
C (19)	69 (6)	48 (6)	34 (5)	19 (4)	3 (4)	11 (5)
C (20)	49 (3)	43 (2)	62 (4)	1 (3)	15 (3)	-17 (2)
C (11A)	36 (2)	42 (3)	28 (3)	-12 (2)	8 (2)	5 (2)
C (12A)	31 (2)	38 (3)	27 (4)	-7 (2)	9 (2)	0 (2)
C (13A)	31 (5)	44 (5)	22 (2)	1 (2)	4 (3)	9 (4)
C (14A)	43 (6)	23 (4)	51 (7)	13 (4)	27 (5)	2 (3)
C (15A)	23 (3)	39 (4)	44 (3)	-3 (2)	13 (2)	5 (2)
C (16A)	36 (4)	84 (6)	35 (4)	-3 (3)	0 (3)	2 (3)
C (17A)	52 (6)	105 (8)	59 (4)	31 (4)	4 (4)	-7 (5)
C (18A)	34 (5)	46 (4)	44 (5)	-17 (3)	0 (3)	-10 (3)
C (19A)	66 (6)	53 (7)	60 (7)	-4 (5)	27 (5)	-4 (4)
C (20A)	71 (6)	113 (9)	70 (5)	-16 (4)	8 (4)	-30 (6)

L2412-6

Table 5. Torsion angles [$^{\circ}$] for 95144.

C(15)-Ti(1)-C(11)-C(12)	-108.8(7)	C(12)-Ti(1)-C(11)-C(12)	0.0
C(16)-Ti(1)-C(11)-C(12)	125.4(10)	C(11A)-Ti(1)-C(11)-C(12)	-57.1(11)
C(15A)-Ti(1)-C(11)-C(12)	37.7(9)	C(12A)-Ti(1)-C(11)-C(12)	-153.5(10)
C(13A)-Ti(1)-C(11)-C(12)	148.2(8)	C(14A)-Ti(1)-C(11)-C(12)	94.5(6)
C(14)-Ti(1)-C(11)-C(12)	-72.8(5)	C(13)-Ti(1)-C(11)-C(12)	-34.5(5)
C(15)-Ti(1)-C(11)-C(16)	125.8(10)	C(12)-Ti(1)-C(11)-C(16)	-125.4(10)
C(16)-Ti(1)-C(11)-C(16)	0.000(3)	C(11A)-Ti(1)-C(11)-C(16)	177.4(11)
C(15A)-Ti(1)-C(11)-C(16)	-87.7(10)	C(12A)-Ti(1)-C(11)-C(16)	81.0(10)
C(13A)-Ti(1)-C(11)-C(16)	22.8(11)	C(14A)-Ti(1)-C(11)-C(16)	-31.0(10)
C(14)-Ti(1)-C(11)-C(16)	161.7(9)	C(13)-Ti(1)-C(11)-C(16)	-159.9(9)
C(15)-Ti(1)-C(11)-C(15)	0.000(2)	C(12)-Ti(1)-C(11)-C(15)	108.8(7)
C(16)-Ti(1)-C(11)-C(15)	-125.8(10)	C(11A)-Ti(1)-C(11)-C(15)	51.7(12)
C(15A)-Ti(1)-C(11)-C(15)	146.5(10)	C(12A)-Ti(1)-C(11)-C(15)	-44.7(8)
C(13A)-Ti(1)-C(11)-C(15)	-103.0(8)	C(14A)-Ti(1)-C(11)-C(15)	-156.7(6)
C(14)-Ti(1)-C(11)-C(15)	36.0(5)	C(13)-Ti(1)-C(11)-C(15)	74.3(6)
C(16)-C(11)-C(12)-C(13)	135.6(12)	C(15)-C(11)-C(12)-C(13)	-4.5(10)
Ti(1)-C(11)-C(12)-C(13)	67.6(9)	C(16)-C(11)-C(12)-C(17)	-34.7(13)
C(15)-C(11)-C(12)-C(17)	-174.8(10)	Ti(1)-C(11)-C(12)-C(17)	-102.7(10)
C(16)-C(11)-C(12)-Ti(1)	68.0(9)	C(15)-C(11)-C(12)-Ti(1)	-72.1(4)
Ti(1)-C(11)-C(12)-Ti(1)	0.0	C(11)-Ti(1)-C(12)-C(13)	-118.6(9)
C(15)-Ti(1)-C(12)-C(13)	-75.7(8)	C(16)-Ti(1)-C(12)-C(13)	-151.9(9)
C(11A)-Ti(1)-C(12)-C(13)	42.2(8)	C(15A)-Ti(1)-C(12)-C(13)	81.3(8)
C(12A)-Ti(1)-C(12)-C(13)	11(2)	C(13A)-Ti(1)-C(12)-C(13)	150(2)
C(14A)-Ti(1)-C(12)-C(13)	118.3(8)	C(14)-Ti(1)-C(12)-C(13)	-33.7(7)
C(13)-Ti(1)-C(12)-C(13)	0.000(4)	C(11)-Ti(1)-C(12)-C(11)	0.0
C(15)-Ti(1)-C(12)-C(11)	43.0(5)	C(16)-Ti(1)-C(12)-C(11)	-33.2(6)
C(11A)-Ti(1)-C(12)-C(11)	160.8(4)	C(15A)-Ti(1)-C(12)-C(11)	-160.0(5)
C(12A)-Ti(1)-C(12)-C(11)	129.3(13)	C(13A)-Ti(1)-C(12)-C(11)	-91.1(13)
C(14A)-Ti(1)-C(12)-C(11)	-123.0(5)	C(14)-Ti(1)-C(12)-C(11)	84.9(5)
C(13)-Ti(1)-C(12)-C(11)	118.6(9)	C(11)-Ti(1)-C(12)-C(17)	121.2(11)
C(15)-Ti(1)-C(12)-C(17)	164.2(10)	C(16)-Ti(1)-C(12)-C(17)	88.0(10)
C(11A)-Ti(1)-C(12)-C(17)	-78.0(10)	C(15A)-Ti(1)-C(12)-C(17)	-38.8(10)
C(12A)-Ti(1)-C(12)-C(17)	-110(2)	C(13A)-Ti(1)-C(12)-C(17)	30(2)
C(14A)-Ti(1)-C(12)-C(17)	-1.9(10)	C(14)-Ti(1)-C(12)-C(17)	-153.9(10)
C(13)-Ti(1)-C(12)-C(17)	-120.2(12)	C(11)-C(12)-C(13)-C(14)	2.2(14)
C(17)-C(12)-C(13)-C(14)	173.2(11)	Ti(1)-C(12)-C(13)-C(14)	59.8(10)
C(11)-C(12)-C(13)-C(18)	176(2)	C(17)-C(12)-C(13)-C(18)	-13(2)
Ti(1)-C(12)-C(13)-C(18)	-126(2)	C(11)-C(12)-C(13)-Ti(1)	-57.6(6)
C(17)-C(12)-C(13)-Ti(1)	113.4(10)	Ti(1)-C(12)-C(13)-Ti(1)	0.000(2)
C(11)-Ti(1)-C(13)-C(12)	38.2(6)	C(15)-Ti(1)-C(13)-C(12)	83.4(8)
C(12)-Ti(1)-C(13)-C(12)	0.000(3)	C(16)-Ti(1)-C(13)-C(12)	25.8(8)
C(11A)-Ti(1)-C(13)-C(12)	-148.6(6)	C(15A)-Ti(1)-C(13)-C(12)	-111.9(7)
C(12A)-Ti(1)-C(13)-C(12)	-176.1(7)	C(13A)-Ti(1)-C(13)-C(12)	-147(2)
C(14A)-Ti(1)-C(13)-C(12)	-94.0(9)	C(14)-Ti(1)-C(13)-C(12)	121.6(11)
C(11)-Ti(1)-C(13)-C(14)	-83.4(7)	C(15)-Ti(1)-C(13)-C(14)	-38.1(6)
C(12)-Ti(1)-C(13)-C(14)	-121.6(11)	C(16)-Ti(1)-C(13)-C(14)	-95.7(8)
C(11A)-Ti(1)-C(13)-C(14)	89.9(7)	C(15A)-Ti(1)-C(13)-C(14)	126.6(7)
C(12A)-Ti(1)-C(13)-C(14)	62.4(9)	C(13A)-Ti(1)-C(13)-C(14)	91(2)
C(14A)-Ti(1)-C(13)-C(14)	144.4(8)	C(14)-Ti(1)-C(13)-C(14)	0.000(2)
C(11)-Ti(1)-C(13)-C(18)	162.6(14)	C(15)-Ti(1)-C(13)-C(18)	-152(2)
C(12)-Ti(1)-C(13)-C(18)	124(2)	C(16)-Ti(1)-C(13)-C(18)	150.3(13)
C(11A)-Ti(1)-C(13)-C(18)	-24.1(13)	C(15A)-Ti(1)-C(13)-C(18)	12.6(14)
C(12A)-Ti(1)-C(13)-C(18)	-52(2)	C(13A)-Ti(1)-C(13)-C(18)	-23(3)
C(14A)-Ti(1)-C(13)-C(18)	30(2)	C(14)-Ti(1)-C(13)-C(18)	-114(2)
C(12)-C(13)-C(14)-C(15)	1.0(13)	C(18)-C(13)-C(14)-C(15)	-173.9(13)
Ti(1)-C(13)-C(14)-C(15)	56.2(6)	C(12)-C(13)-C(14)-C(19)	171.1(12)
C(18)-C(13)-C(14)-C(19)	-4(2)	Ti(1)-C(13)-C(14)-C(19)	-133.8(13)
C(12)-C(13)-C(14)-Ti(1)	-55.2(9)	C(18)-C(13)-C(14)-Ti(1)	130(2)
Ti(1)-C(13)-C(14)-Ti(1)	0.0	C(11)-Ti(1)-C(14)-C(13)	78.0(8)

L 2412-7

C(15)-Ti(1)-C(14)-C(13)	116.9(10)	C(12)-Ti(1)-C(14)-C(13)	34.4(7)
C(16)-Ti(1)-C(14)-C(13)	89.3(9)	C(11A)-Ti(1)-C(14)-C(13)	-97.3(8)
C(15A)-Ti(1)-C(14)-C(13)	-67.5(8)	C(12A)-Ti(1)-C(14)-C(13)	-133.4(8)
C(13A)-Ti(1)-C(14)-C(13)	-147.9(13)	C(14A)-Ti(1)-C(14)-C(13)	-81.1(13)
C(13)-Ti(1)-C(14)-C(13)	0.000(1)	C(11)-Ti(1)-C(14)-C(15)	-38.8(5)
C(15)-Ti(1)-C(14)-C(15)	0.000(2)	C(12)-Ti(1)-C(14)-C(15)	-82.5(6)
C(16)-Ti(1)-C(14)-C(15)	-27.5(8)	C(11A)-Ti(1)-C(14)-C(15)	145.9(6)
C(15A)-Ti(1)-C(14)-C(15)	175.6(7)	C(12A)-Ti(1)-C(14)-C(15)	109.8(6)
C(13A)-Ti(1)-C(14)-C(15)	95.3(9)	C(14A)-Ti(1)-C(14)-C(15)	162.0(9)
C(13)-Ti(1)-C(14)-C(15)	-116.9(10)	C(11)-Ti(1)-C(14)-C(19)	-148.4(11)
C(15)-Ti(1)-C(14)-C(19)	-109.6(12)	C(12)-Ti(1)-C(14)-C(19)	167.9(12)
C(16)-Ti(1)-C(14)-C(19)	-137.1(11)	C(11A)-Ti(1)-C(14)-C(19)	36.3(11)
C(15A)-Ti(1)-C(14)-C(19)	66.0(11)	C(12A)-Ti(1)-C(14)-C(19)	0.2(11)
C(13A)-Ti(1)-C(14)-C(19)	-14.3(14)	C(14A)-Ti(1)-C(14)-C(19)	52(2)
C(13)-Ti(1)-C(14)-C(19)	133.6(14)	C(12)-C(11)-C(15)-C(14)	5.2(8)
C(16)-C(11)-C(15)-C(14)	-135.1(9)	Ti(1)-C(11)-C(15)-C(14)	-68.0(6)
C(12)-C(11)-C(15)-C(20)	176.2(8)	C(16)-C(11)-C(15)-C(20)	36.0(11)
Ti(1)-C(11)-C(15)-C(20)	103.1(8)	C(12)-C(11)-C(15)-Ti(1)	73.2(4)
C(16)-C(11)-C(15)-Ti(1)	-67.1(7)	Ti(1)-C(11)-C(15)-Ti(1)	0.000(2)
C(13)-C(14)-C(15)-C(11)	-3.9(11)	C(19)-C(14)-C(15)-C(11)	-175.3(9)
Ti(1)-C(14)-C(15)-C(11)	58.4(5)	C(13)-C(14)-C(15)-C(20)	-174.2(11)
C(19)-C(14)-C(15)-C(20)	14(2)	Ti(1)-C(14)-C(15)-C(20)	-112.0(10)
C(13)-C(14)-C(15)-Ti(1)	-62.3(9)	C(19)-C(14)-C(15)-Ti(1)	126.3(10)
Ti(1)-C(14)-C(15)-Ti(1)	0.000(2)	C(11)-Ti(1)-C(15)-C(11)	0.000(2)
C(12)-Ti(1)-C(15)-C(11)	-41.9(4)	C(16)-Ti(1)-C(15)-C(11)	32.8(6)
C(11A)-Ti(1)-C(15)-C(11)	-162.6(4)	C(15A)-Ti(1)-C(15)-C(11)	-128.0(12)
C(12A)-Ti(1)-C(15)-C(11)	156.8(4)	C(13A)-Ti(1)-C(15)-C(11)	118.0(6)
C(14A)-Ti(1)-C(15)-C(11)	91.4(13)	C(14)-Ti(1)-C(15)-C(11)	-117.5(8)
C(13)-Ti(1)-C(15)-C(11)	-81.9(6)	C(11)-Ti(1)-C(15)-C(14)	117.5(8)
C(12)-Ti(1)-C(15)-C(14)	75.6(6)	C(16)-Ti(1)-C(15)-C(14)	150.3(8)
C(11A)-Ti(1)-C(15)-C(14)	-45.1(7)	C(15A)-Ti(1)-C(15)-C(14)	-11(2)
C(12A)-Ti(1)-C(15)-C(14)	-85.7(7)	C(13A)-Ti(1)-C(15)-C(14)	-124.5(8)
C(14A)-Ti(1)-C(15)-C(14)	-151(2)	C(14)-Ti(1)-C(15)-C(14)	0.000(3)
C(13)-Ti(1)-C(15)-C(14)	35.6(6)	C(11)-Ti(1)-C(15)-C(20)	-115.4(10)
C(12)-Ti(1)-C(15)-C(20)	-157.3(9)	C(16)-Ti(1)-C(15)-C(20)	-82.5(10)
C(11A)-Ti(1)-C(15)-C(20)	82.0(9)	C(15A)-Ti(1)-C(15)-C(20)	116.7(13)
C(12A)-Ti(1)-C(15)-C(20)	41.4(9)	C(13A)-Ti(1)-C(15)-C(20)	2.6(11)
C(14A)-Ti(1)-C(15)-C(20)	-24(2)	C(14)-Ti(1)-C(15)-C(20)	127.1(11)
C(13)-Ti(1)-C(15)-C(20)	162.7(10)	C(12)-C(11)-C(16)-Ti(1)	-67.8(7)
C(15)-C(11)-C(16)-Ti(1)	66.2(6)	Ti(1)-C(11)-C(16)-Ti(1)	0.000(3)
C(11)-Ti(1)-C(16)-C(11)	0.000(3)	C(15)-Ti(1)-C(16)-C(11)	-33.6(6)
C(12)-Ti(1)-C(16)-C(11)	33.2(6)	C(11A)-Ti(1)-C(16)-C(11)	-177.9(9)
C(15A)-Ti(1)-C(16)-C(11)	137.5(5)	C(12A)-Ti(1)-C(16)-C(11)	-140.4(6)
C(13A)-Ti(1)-C(16)-C(11)	-164.6(7)	C(14A)-Ti(1)-C(16)-C(11)	159.6(6)
C(14)-Ti(1)-C(16)-C(11)	-16.4(8)	C(13)-Ti(1)-C(16)-C(11)	17.6(8)
C(11)-Ti(1)-C(11A)-C(15A)	120.6(10)	C(15)-Ti(1)-C(11A)-C(15A)	159.9(8)
C(12)-Ti(1)-C(11A)-C(15A)	77.5(6)	C(16)-Ti(1)-C(11A)-C(15A)	-64(2)
C(15A)-Ti(1)-C(11A)-C(15A)	0.000(3)	C(12A)-Ti(1)-C(11A)-C(15A)	-117.4(7)
C(13A)-Ti(1)-C(11A)-C(15A)	-79.2(6)	C(14A)-Ti(1)-C(11A)-C(15A)	-37.5(5)
C(14)-Ti(1)-C(11A)-C(15A)	134.8(6)	C(13)-Ti(1)-C(11A)-C(15A)	100.4(6)
C(11)-Ti(1)-C(11A)-C(12A)	-122.0(10)	C(15)-Ti(1)-C(11A)-C(12A)	-82.7(6)
C(12)-Ti(1)-C(11A)-C(12A)	-165.1(8)	C(16)-Ti(1)-C(11A)-C(12A)	54(2)
C(15A)-Ti(1)-C(11A)-C(12A)	117.4(7)	C(12A)-Ti(1)-C(11A)-C(12A)	0.0
C(13A)-Ti(1)-C(11A)-C(12A)	38.2(6)	C(14A)-Ti(1)-C(11A)-C(12A)	79.9(6)
C(14)-Ti(1)-C(11A)-C(12A)	-107.8(6)	C(13)-Ti(1)-C(11A)-C(12A)	-142.2(7)
C(11)-Ti(1)-C(11A)-C(16A)	-1(2)	C(15)-Ti(1)-C(11A)-C(16A)	38.8(11)
C(12)-Ti(1)-C(11A)-C(16A)	-43.6(11)	C(16)-Ti(1)-C(11A)-C(16A)	175(2)
C(15A)-Ti(1)-C(11A)-C(16A)	-121.1(11)	C(12A)-Ti(1)-C(11A)-C(16A)	121.5(11)
C(13A)-Ti(1)-C(11A)-C(16A)	159.7(11)	C(14A)-Ti(1)-C(11A)-C(16A)	-158.6(10)
C(14)-Ti(1)-C(11A)-C(16A)	13.7(10)	C(13)-Ti(1)-C(11A)-C(16A)	-20.7(10)
C(15A)-C(11A)-C(12A)-C(13A)	-1.4(10)	C(16A)-C(11A)-C(12A)-C(13A)	177.0(12)
Ti(1)-C(11A)-C(12A)-C(13A)	-65.5(9)	C(15A)-C(11A)-C(12A)-C(17A)	-171.1(11)
C(16A)-C(11A)-C(12A)-C(17A)	7.4(14)	Ti(1)-C(11A)-C(12A)-C(17A)	124.9(11)

L2412-8

C(15A)-C(11A)-C(12A)-Ti(1)	64.1(4)	C(16A)-C(11A)-C(12A)-Ti(1)	-117.5(9)
Ti(1)-C(11A)-C(12A)-Ti(1)	0.0	C(11)-Ti(1)-C(12A)-C(13A)	-96.4(9)
C(15)-Ti(1)-C(12A)-C(13A)	-126.1(8)	C(12)-Ti(1)-C(12A)-C(13A)	156.5(14)
C(16)-Ti(1)-C(12A)-C(13A)	-44.4(10)	C(11A)-Ti(1)-C(12A)-C(13A)	113.8(9)
C(15A)-Ti(1)-C(12A)-C(13A)	77.1(8)	C(13A)-Ti(1)-C(12A)-C(13A)	0.000(4)
C(14A)-Ti(1)-C(12A)-C(13A)	37.7(7)	C(14)-Ti(1)-C(12A)-C(13A)	-164.5(8)
C(13)-Ti(1)-C(12A)-C(13A)	164.2(11)	C(11)-Ti(1)-C(12A)-C(11A)	149.8(6)
C(15)-Ti(1)-C(12A)-C(11A)	120.1(5)	C(12)-Ti(1)-C(12A)-C(11A)	43(2)
C(16)-Ti(1)-C(12A)-C(11A)	-158.3(6)	C(11A)-Ti(1)-C(12A)-C(11A)	0.0
C(15A)-Ti(1)-C(12A)-C(11A)	-36.7(5)	C(13A)-Ti(1)-C(12A)-C(11A)	-113.8(9)
C(14A)-Ti(1)-C(12A)-C(11A)	-76.1(5)	C(14)-Ti(1)-C(12A)-C(11A)	81.7(5)
C(13)-Ti(1)-C(12A)-C(11A)	50.3(8)	C(11)-Ti(1)-C(12A)-C(17A)	30.9(14)
C(15)-Ti(1)-C(12A)-C(17A)	1.2(12)	C(12)-Ti(1)-C(12A)-C(17A)	-76(2)
C(16)-Ti(1)-C(12A)-C(17A)	82.9(12)	C(11A)-Ti(1)-C(12A)-C(17A)	-118.9(13)
C(15A)-Ti(1)-C(12A)-C(17A)	-155.6(12)	C(13A)-Ti(1)-C(12A)-C(17A)	127.3(14)
C(14A)-Ti(1)-C(12A)-C(17A)	165.1(12)	C(14)-Ti(1)-C(12A)-C(17A)	-37.2(11)
C(13)-Ti(1)-C(12A)-C(17A)	-68.5(12)	C(11A)-C(12A)-C(13A)-C(14A)	-0.6(14)
C(17A)-C(12A)-C(13A)-C(14A)	168.3(12)	Ti(1)-C(12A)-C(13A)-C(14A)	-65.0(10)
C(11A)-C(12A)-C(13A)-C(18A)	-179.9(12)	C(17A)-C(12A)-C(13A)-C(18A)	-11(2)
Ti(1)-C(12A)-C(13A)-C(18A)	116(2)	C(11A)-C(12A)-C(13A)-Ti(1)	64.4(5)
C(17A)-C(12A)-C(13A)-Ti(1)	-126.7(13)	Ti(1)-C(12A)-C(13A)-Ti(1)	0.000(3)
C(11)-Ti(1)-C(13A)-C(12A)	132.4(6)	C(15)-Ti(1)-C(13A)-C(12A)	76.7(9)
C(12)-Ti(1)-C(13A)-C(12A)	-161.1(10)	C(16)-Ti(1)-C(13A)-C(12A)	146.5(8)
C(11A)-Ti(1)-C(13A)-C(12A)	-39.1(6)	C(15A)-Ti(1)-C(13A)-C(12A)	-81.2(7)
C(12A)-Ti(1)-C(13A)-C(12A)	0.000(5)	C(14A)-Ti(1)-C(13A)-C(12A)	-115.1(11)
C(14)-Ti(1)-C(13A)-C(12A)	24.4(12)	C(13)-Ti(1)-C(13A)-C(12A)	-40(3)
C(11)-Ti(1)-C(13A)-C(14A)	-112.6(7)	C(15)-Ti(1)-C(13A)-C(14A)	-168.3(6)
C(12)-Ti(1)-C(13A)-C(14A)	-46(2)	C(16)-Ti(1)-C(13A)-C(14A)	-98.5(8)
C(11A)-Ti(1)-C(13A)-C(14A)	76.0(7)	C(15A)-Ti(1)-C(13A)-C(14A)	33.9(6)
C(12A)-Ti(1)-C(13A)-C(14A)	115.1(11)	C(14A)-Ti(1)-C(13A)-C(14A)	0.000(1)
C(14)-Ti(1)-C(13A)-C(14A)	139.4(8)	C(13)-Ti(1)-C(13A)-C(14A)	75(2)
C(11)-Ti(1)-C(13A)-C(18A)	15.6(14)	C(15)-Ti(1)-C(13A)-C(18A)	-40.1(13)
C(12)-Ti(1)-C(13A)-C(18A)	82(2)	C(16)-Ti(1)-C(13A)-C(18A)	29.7(12)
C(11A)-Ti(1)-C(13A)-C(18A)	-155.8(12)	C(15A)-Ti(1)-C(13A)-C(18A)	162.0(13)
C(12A)-Ti(1)-C(13A)-C(18A)	-116.8(14)	C(14A)-Ti(1)-C(13A)-C(18A)	128.2(14)
C(14)-Ti(1)-C(13A)-C(18A)	-92.4(12)	C(13)-Ti(1)-C(13A)-C(18A)	-157.2(14)
C(12A)-C(13A)-C(14A)-C(15A)	3(2)	C(18A)-C(13A)-C(14A)-C(15A)	-178(2)
Ti(1)-C(13A)-C(14A)-C(15A)	-61.7(8)	C(12A)-C(13A)-C(14A)-C(19A)	178.3(11)
C(18A)-C(13A)-C(14A)-C(19A)	-2(2)	Ti(1)-C(13A)-C(14A)-C(19A)	114.1(9)
C(12A)-C(13A)-C(14A)-Ti(1)	64.2(10)	C(18A)-C(13A)-C(14A)-Ti(1)	-117(2)
Ti(1)-C(13A)-C(14A)-Ti(1)	0.0	C(11)-Ti(1)-C(14A)-C(15A)	-130.4(6)
C(15)-Ti(1)-C(14A)-C(15A)	156(2)	C(12)-Ti(1)-C(14A)-C(15A)	-78.4(7)
C(16)-Ti(1)-C(14A)-C(15A)	-149.5(7)	C(11A)-Ti(1)-C(14A)-C(15A)	39.9(5)
C(15A)-Ti(1)-C(14A)-C(15A)	0.000(4)	C(12A)-Ti(1)-C(14A)-C(15A)	82.7(6)
C(13A)-Ti(1)-C(14A)-C(15A)	120.7(9)	C(14)-Ti(1)-C(14A)-C(15A)	21(2)
C(13)-Ti(1)-C(14A)-C(15A)	-32.1(9)	C(11)-Ti(1)-C(14A)-C(13A)	108.9(7)
C(15)-Ti(1)-C(14A)-C(13A)	36(2)	C(12)-Ti(1)-C(14A)-C(13A)	160.9(8)
C(16)-Ti(1)-C(14A)-C(13A)	89.8(9)	C(11A)-Ti(1)-C(14A)-C(13A)	-80.8(7)
C(15A)-Ti(1)-C(14A)-C(13A)	-120.7(9)	C(12A)-Ti(1)-C(14A)-C(13A)	-37.9(7)
C(13A)-Ti(1)-C(14A)-C(13A)	0.000(1)	C(14)-Ti(1)-C(14A)-C(13A)	-99.9(13)
C(13)-Ti(1)-C(14A)-C(13A)	-152.8(12)	C(11)-Ti(1)-C(14A)-C(19A)	-2.5(11)
C(15)-Ti(1)-C(14A)-C(19A)	-76(2)	C(12)-Ti(1)-C(14A)-C(19A)	49.5(10)
C(16)-Ti(1)-C(14A)-C(19A)	-21.6(10)	C(11A)-Ti(1)-C(14A)-C(19A)	167.7(10)
C(15A)-Ti(1)-C(14A)-C(19A)	127.9(11)	C(12A)-Ti(1)-C(14A)-C(19A)	-149.4(10)
C(13A)-Ti(1)-C(14A)-C(19A)	-111.4(12)	C(14)-Ti(1)-C(14A)-C(19A)	148.6(12)
C(13)-Ti(1)-C(14A)-C(19A)	95.8(11)	C(13A)-C(14A)-C(15A)-C(11A)	-3.4(12)
C(19A)-C(14A)-C(15A)-C(11A)	-178.4(11)	Ti(1)-C(14A)-C(15A)-C(11A)	-65.0(5)
C(13A)-C(14A)-C(15A)-C(20A)	-178.5(12)	C(19A)-C(14A)-C(15A)-C(20A)	6(2)
Ti(1)-C(14A)-C(15A)-C(20A)	119.8(10)	C(13A)-C(14A)-C(15A)-Ti(1)	61.6(10)
C(19A)-C(14A)-C(15A)-Ti(1)	-113.4(12)	Ti(1)-C(14A)-C(15A)-Ti(1)	0.000(2)
C(12A)-C(11A)-C(15A)-C(14A)	2.9(8)	C(16A)-C(11A)-C(15A)-C(14A)	-175.5(10)
Ti(1)-C(11A)-C(15A)-C(14A)	66.9(6)	C(12A)-C(11A)-C(15A)-C(20A)	177.8(10)
C(16A)-C(11A)-C(15A)-C(20A)	-0.7(14)	Ti(1)-C(11A)-C(15A)-C(20A)	-118.3(10)

L2412-9

C(12A)-C(11A)-C(15A)-Ti(1)	-63.9(4)	C(16A)-C(11A)-C(15A)-Ti(1)	117.6(9)
Ti(1)-C(11A)-C(15A)-Ti(1)	0.000(1)	C(11)-Ti(1)-C(15A)-C(14A)	97.2(7)
C(15)-Ti(1)-C(15A)-C(14A)	-162.7(11)	C(12)-Ti(1)-C(15A)-C(14A)	122.0(6)
C(16)-Ti(1)-C(15A)-C(14A)	41.4(9)	C(11A)-Ti(1)-C(15A)-C(14A)	-113.2(7)
C(12A)-Ti(1)-C(15A)-C(14A)	-76.3(6)	C(13A)-Ti(1)-C(15A)-C(14A)	-35.2(6)
C(14A)-Ti(1)-C(15A)-C(14A)	0.000(4)	C(14)-Ti(1)-C(15A)-C(14A)	-170.1(7)
C(13)-Ti(1)-C(15A)-C(14A)	157.6(7)	C(11)-Ti(1)-C(15A)-C(11A)	-149.5(6)
C(15)-Ti(1)-C(15A)-C(11A)	-50(2)	C(12)-Ti(1)-C(15A)-C(11A)	-124.8(5)
C(16)-Ti(1)-C(15A)-C(11A)	154.6(7)	C(11A)-Ti(1)-C(15A)-C(11A)	0.000(3)
C(12A)-Ti(1)-C(15A)-C(11A)	36.9(4)	C(13A)-Ti(1)-C(15A)-C(11A)	78.0(6)
C(14A)-Ti(1)-C(15A)-C(11A)	113.2(7)	C(14)-Ti(1)-C(15A)-C(11A)	-56.8(6)
C(13)-Ti(1)-C(15A)-C(11A)	-89.2(6)	C(11)-Ti(1)-C(15A)-C(20A)	-23.5(14)
C(15)-Ti(1)-C(15A)-C(20A)	77(2)	C(12)-Ti(1)-C(15A)-C(20A)	1.3(12)
C(16)-Ti(1)-C(15A)-C(20A)	-79.4(12)	C(11A)-Ti(1)-C(15A)-C(20A)	126.0(12)
C(12A)-Ti(1)-C(15A)-C(20A)	163.0(12)	C(13A)-Ti(1)-C(15A)-C(20A)	-156.0(12)
C(14A)-Ti(1)-C(15A)-C(20A)	-120.7(13)	C(14)-Ti(1)-C(15A)-C(20A)	69.2(11)
C(13)-Ti(1)-C(15A)-C(20A)	36.9(11)		

Symmetry transformations used to generate equivalent atoms:

L2412-10 |

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 95144.

	x	y	z	U(eq)
H(16B)	1413 (12)	1140 (16)	2780 (11)	57
H(16C)	2050 (12)	2468 (16)	2496 (11)	57
H(17A)	4275 (27)	3037 (14)	2881 (19)	104
H(17B)	4625 (20)	3754 (23)	3961 (16)	104
H(17C)	3515 (14)	3970 (21)	3311 (27)	104
H(18A)	5654 (9)	1968 (31)	5551 (17)	95
H(18B)	5066 (17)	1943 (32)	6436 (10)	95
H(18C)	5038 (15)	3280 (14)	5754 (21)	95
H(19A)	4179 (22)	-1078 (20)	6172 (11)	77
H(19B)	3161 (11)	-549 (29)	6410 (15)	77
H(19C)	4175 (23)	258 (16)	6849 (9)	77
H(20A)	2155 (14)	-1581 (17)	3942 (19)	76
H(20B)	1385 (10)	-374 (14)	3984 (25)	76
H(20C)	1971 (18)	-1087 (25)	5006 (10)	76
H(16D)	2777 (15)	3750 (24)	7670 (12)	79
H(16E)	3629 (11)	3457 (38)	7075 (13)	79
H(16F)	2955 (21)	2230 (17)	7316 (16)	79
H(17G)	431 (23)	2049 (18)	6677 (24)	110
H(17H)	1488 (13)	1299 (35)	6914 (23)	110
H(17I)	655 (26)	882 (21)	5936 (15)	110
H(18G)	-629 (9)	3517 (14)	4184 (17)	64
H(18H)	-328 (12)	1991 (18)	4551 (12)	64
H(18I)	-47 (9)	2572 (26)	3552 (9)	64
H(19G)	419 (13)	5504 (31)	3672 (16)	86
H(19H)	1191 (28)	4698 (19)	3169 (10)	86
H(19I)	1523 (19)	6078 (23)	3784 (14)	86
H(20G)	2798 (15)	6455 (15)	5669 (29)	129
H(20H)	3256 (25)	5645 (30)	4859 (16)	129
H(20I)	3652 (16)	5342 (24)	6039 (25)	129